



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:28 AM UTC

PDB ID : 9LBY / pdb_00009lby
Title : Crystal Structure of Maize Lipoxygenase3
Authors : Zhang, X.
Deposited on : 2025-01-03
Resolution : 2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

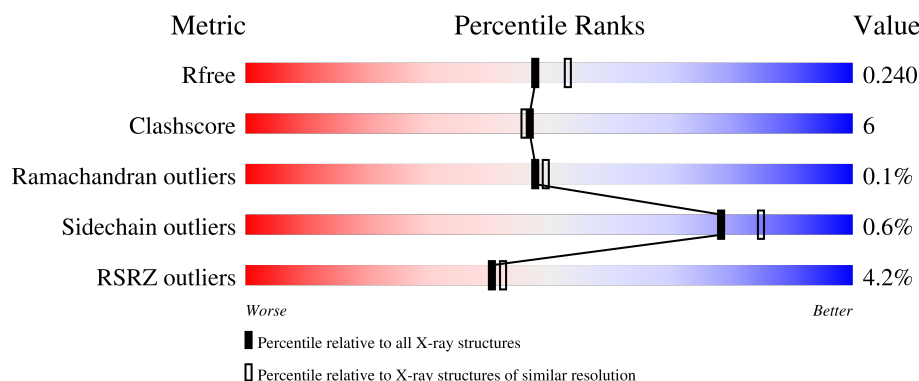
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	873	<div> <div>4%</div> <div>81% 12% 7%</div> </div>
1	B	873	<div> <div>3%</div> <div>81% 13% 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14339 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	823	Total	C	N	O	S	0	0	0
			6513	4150	1125	1223	15			
1	A	810	Total	C	N	O	S	0	0	0
			6415	4087	1111	1202	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	initiating methionine	UNP Q8W0V2
B	-7	SER	-	expression tag	UNP Q8W0V2
B	-6	HIS	-	expression tag	UNP Q8W0V2
B	-5	HIS	-	expression tag	UNP Q8W0V2
B	-4	HIS	-	expression tag	UNP Q8W0V2
B	-3	HIS	-	expression tag	UNP Q8W0V2
B	-2	HIS	-	expression tag	UNP Q8W0V2
B	-1	HIS	-	expression tag	UNP Q8W0V2
B	0	SER	-	expression tag	UNP Q8W0V2
B	715	LEU	PHE	conflict	UNP Q8W0V2
A	-8	MET	-	initiating methionine	UNP Q8W0V2
A	-7	SER	-	expression tag	UNP Q8W0V2
A	-6	HIS	-	expression tag	UNP Q8W0V2
A	-5	HIS	-	expression tag	UNP Q8W0V2
A	-4	HIS	-	expression tag	UNP Q8W0V2
A	-3	HIS	-	expression tag	UNP Q8W0V2
A	-2	HIS	-	expression tag	UNP Q8W0V2
A	-1	HIS	-	expression tag	UNP Q8W0V2
A	0	SER	-	expression tag	UNP Q8W0V2
A	715	LEU	PHE	conflict	UNP Q8W0V2

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Fe 1	0	0
2	A	1	Total 1	Fe 1	0	0

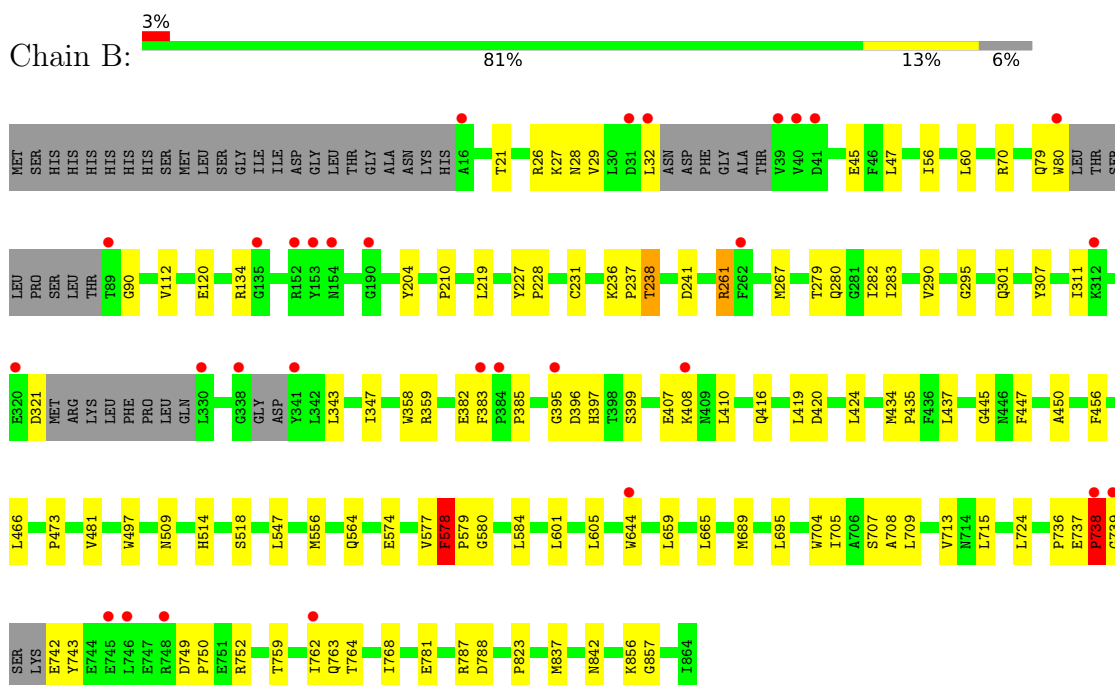
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	739	Total 739	O 739	0	0
3	A	670	Total 670	O 670	0	0

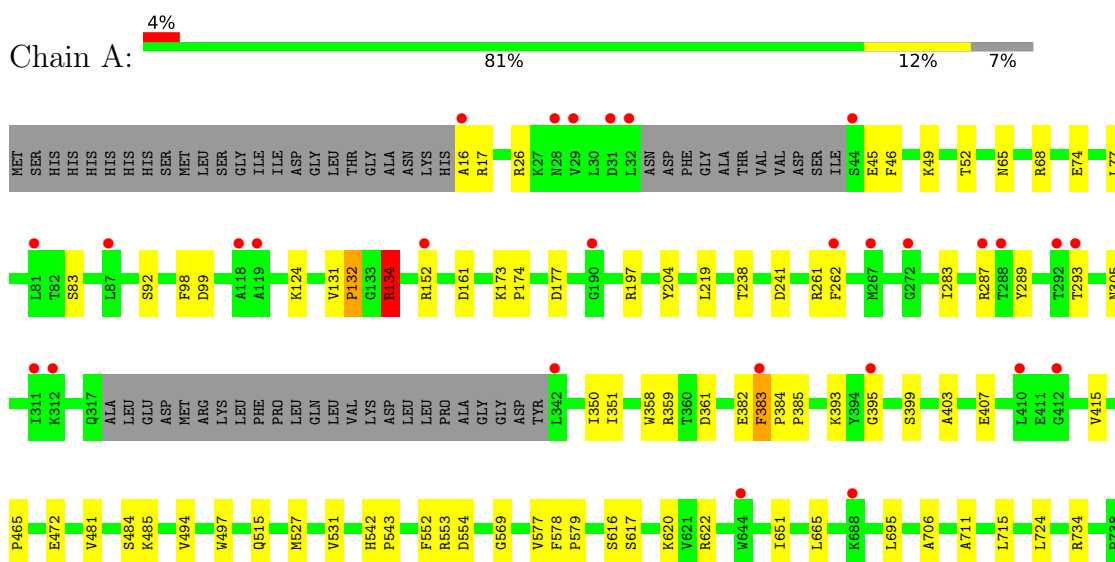
3 Residue-property plots [i](#)

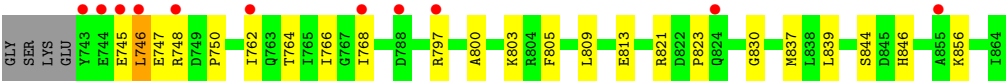
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lipoxxygenase



• Molecule 1: Lipoxxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.51Å 75.04Å 107.72Å 98.91° 101.88° 113.71°	Depositor
Resolution (Å)	27.36 – 2.08 27.36 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.0 (27.36-2.08) 97.0 (27.36-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.197 , 0.242 0.197 , 0.240	Depositor DCC
R_{free} test set	5267 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14339	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	4/6580 (0.1%)	0.72	17/8956 (0.2%)
1	B	0.63	5/6677 (0.1%)	0.82	20/9084 (0.2%)
All	All	0.58	9/13257 (0.1%)	0.77	37/18040 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	PRO	N-CA	18.84	1.69	1.47
1	B	237	PRO	N-CA	15.70	1.66	1.47
1	A	384	PRO	C-N	14.06	1.50	1.33
1	A	131	VAL	C-N	8.91	1.44	1.33
1	B	236	LYS	C-N	7.58	1.43	1.33
1	B	473	PRO	C-O	-6.27	1.16	1.23
1	A	383	PHE	C-O	-5.75	1.16	1.24
1	B	435	PRO	C-O	-5.38	1.17	1.24
1	B	736	PRO	C-O	-5.16	1.18	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	LYS	CA-C-N	16.03	136.25	119.89
1	B	236	LYS	C-N-CA	16.03	136.25	119.89
1	A	131	VAL	CA-C-N	14.70	135.66	119.93
1	A	131	VAL	C-N-CA	14.70	135.66	119.93
1	A	384	PRO	N-CA-C	-10.20	98.25	110.70
1	A	383	PHE	CA-C-O	-9.69	106.89	120.16
1	A	132	PRO	N-CA-C	-8.72	97.05	111.26
1	A	384	PRO	CA-C-N	8.65	129.18	119.83
1	A	384	PRO	C-N-CA	8.65	129.18	119.83
1	B	578	PHE	CB-CG-CD2	-8.24	106.68	120.70
1	B	383	PHE	N-CA-CB	8.17	118.15	110.39
1	B	382	GLU	CA-C-N	-7.93	111.03	119.83
1	B	382	GLU	C-N-CA	-7.93	111.03	119.83
1	A	383	PHE	N-CA-CB	7.67	124.02	110.37
1	B	781	GLU	CA-CB-CG	7.22	128.54	114.10
1	B	237	PRO	CA-N-CD	-6.99	102.21	112.00
1	B	237	PRO	N-CA-C	-6.78	100.34	111.11
1	A	746	LEU	CA-C-N	-6.65	109.75	122.53
1	A	746	LEU	C-N-CA	-6.65	109.75	122.53
1	A	132	PRO	CA-N-CD	-6.33	103.13	112.00
1	B	447	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	384	PRO	O-C-N	-5.91	114.48	121.46
1	B	738	PRO	N-CA-CB	-5.77	97.19	103.25
1	B	383	PHE	CB-CA-C	-5.60	104.77	113.57
1	A	134	ARG	CG-CD-NE	-5.48	99.94	112.00
1	B	396	ASP	N-CA-C	-5.40	99.72	108.41
1	B	823	PRO	CA-C-N	-5.39	112.03	122.06
1	B	823	PRO	C-N-CA	-5.39	112.03	122.06
1	A	16	ALA	CA-C-N	-5.37	111.80	121.62
1	A	16	ALA	C-N-CA	-5.37	111.80	121.62
1	A	132	PRO	CB-CA-C	5.35	118.44	111.64
1	B	238	THR	N-CA-CB	-5.32	102.51	110.17
1	A	382	GLU	CA-C-O	-5.28	114.59	120.66
1	B	578	PHE	CB-CA-C	5.19	120.39	110.17
1	B	445	GLY	CA-C-N	-5.09	115.81	122.99
1	B	445	GLY	C-N-CA	-5.09	115.81	122.99
1	B	578	PHE	N-CA-CB	-5.01	101.46	110.37

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	261	ARG	Peptide
1	B	578	PHE	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6415	0	6292	69	0
1	B	6513	0	6382	79	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	670	0	0	12	0
3	B	739	0	0	10	0
All	All	14339	0	12674	147	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PRO:CA	1:A:132:PRO:N	1.69	1.39
1:B:395:GLY:HA3	1:B:481:VAL:HG12	1.44	0.97
1:B:238:THR:HG22	1:B:241:ASP:H	1.31	0.94
1:A:26:ARG:NH1	1:A:45:GLU:OE2	2.06	0.88
1:B:385:PRO:HD2	1:B:399:SER:HB3	1.53	0.87
1:B:32:LEU:HD11	1:B:267:MET:HG3	1.58	0.85
1:A:204:TYR:HB2	1:A:219:LEU:HB2	1.64	0.79
1:A:132:PRO:N	1:A:132:PRO:C	2.42	0.78
1:B:577:VAL:HG12	1:B:579:PRO:HD2	1.66	0.77
1:B:395:GLY:CA	1:B:481:VAL:HG12	2.19	0.72
1:A:124:LYS:NZ	3:A:1001:HOH:O	2.23	0.72
1:B:749:ASP:OD2	1:B:752:ARG:NH1	2.22	0.72
1:A:622:ARG:NH1	3:A:1002:HOH:O	2.23	0.71
1:B:134:ARG:NH1	3:B:1003:HOH:O	2.24	0.70
1:A:395:GLY:HA3	1:A:481:VAL:HG12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:PHE:CD1	1:B:579:PRO:HD3	2.27	0.69
1:A:287:ARG:HD2	1:A:762:ILE:HD13	1.75	0.67
1:A:494:VAL:HB	1:A:747:GLU:HG2	1.78	0.65
1:A:134:ARG:NH1	1:A:161:ASP:OD2	2.29	0.65
1:B:397:HIS:CE1	1:B:434:MET:HE3	2.33	0.64
1:B:307:TYR:HB3	1:B:347:ILE:HD13	1.78	0.64
1:B:601:LEU:HD12	1:B:704:TRP:CH2	2.32	0.63
1:A:472:GLU:OE1	1:A:734:ARG:NH2	2.31	0.63
1:A:577:VAL:HG12	1:A:579:PRO:HD2	1.81	0.63
1:B:385:PRO:HD2	1:B:399:SER:CB	2.27	0.62
1:A:385:PRO:HD2	1:A:399:SER:HB3	1.81	0.62
1:B:514:HIS:HA	1:B:518:SER:HB2	1.82	0.62
1:B:60:LEU:HB3	1:B:70:ARG:HD2	1.81	0.62
1:B:238:THR:CG2	1:B:241:ASP:H	2.09	0.62
1:B:231:CYS:HB2	1:B:556:MET:HE3	1.81	0.62
1:B:578:PHE:HD1	1:B:579:PRO:N	1.97	0.61
1:A:261:ARG:HD2	3:A:1205:HOH:O	1.99	0.61
1:B:301:GLN:NE2	3:B:1011:HOH:O	2.34	0.61
1:A:383:PHE:CG	1:A:415:VAL:HG11	2.36	0.61
1:B:79:GLN:O	1:B:80:TRP:HD1	1.84	0.60
1:B:764:THR:O	1:B:768:ILE:HG12	2.01	0.60
1:B:724:LEU:HD21	1:B:759:THR:HB	1.84	0.59
1:A:803:LYS:NZ	3:A:1015:HOH:O	2.35	0.59
1:B:456:PHE:HB2	1:B:466:LEU:HD11	1.85	0.57
1:B:238:THR:HG22	1:B:241:ASP:N	2.11	0.57
1:A:837:MET:HE3	1:A:856:LYS:HD2	1.86	0.56
1:B:347:ILE:HG12	1:A:616:SER:O	2.05	0.56
1:B:397:HIS:HE1	1:B:434:MET:HE3	1.70	0.55
1:A:238:THR:HG22	1:A:241:ASP:O	2.06	0.55
1:A:52:THR:HB	1:A:74:GLU:HB2	1.87	0.55
1:B:601:LEU:HD23	1:B:605:LEU:HG	1.89	0.54
1:A:484:SER:O	1:A:485:LYS:HD2	2.06	0.54
1:A:173:LYS:HE2	1:A:177:ASP:OD1	2.06	0.54
1:A:17:ARG:HG3	1:A:98:PHE:O	2.08	0.53
1:B:514:HIS:CD2	1:B:713:VAL:HG22	2.44	0.53
1:A:746:LEU:O	1:A:750:PRO:HG3	2.09	0.53
1:A:403:ALA:O	1:A:407:GLU:HB2	2.09	0.53
1:B:564:GLN:HG3	3:B:1324:HOH:O	2.09	0.53
1:A:745:GLU:N	3:A:1004:HOH:O	2.25	0.53
1:B:578:PHE:CD1	1:B:579:PRO:CD	2.92	0.52
1:A:238:THR:HG23	1:A:241:ASP:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:LEU:HD12	1:B:644:TRP:CH2	2.45	0.52
1:A:287:ARG:HD2	1:A:762:ILE:CD1	2.41	0.51
1:A:542:HIS:ND1	1:A:543:PRO:HD2	2.25	0.51
1:A:383:PHE:CD1	1:A:383:PHE:O	2.64	0.51
1:A:665:LEU:HD21	1:A:695:LEU:HD13	1.92	0.51
1:B:578:PHE:CD1	1:B:578:PHE:C	2.89	0.51
1:A:361:ASP:HB3	1:A:465:PRO:HG2	1.92	0.51
1:A:65:ASN:ND2	1:A:68:ARG:HD3	2.26	0.51
1:A:289:TYR:O	1:A:293:THR:HG23	2.11	0.51
1:A:350:ILE:HG23	1:A:351:ILE:HG23	1.92	0.51
1:A:287:ARG:HA	1:A:762:ILE:HD12	1.93	0.50
1:A:651:ILE:HG23	1:A:797:ARG:HD2	1.92	0.50
1:A:724:LEU:HD22	1:A:764:THR:OG1	2.11	0.50
1:B:321:ASP:N	3:B:1021:HOH:O	2.43	0.50
1:A:800:ALA:HA	1:A:803:LYS:HE3	1.93	0.50
1:B:689:MET:HE1	1:B:695:LEU:HA	1.94	0.49
1:B:787:ARG:HD3	3:B:1001:HOH:O	2.11	0.49
1:A:68:ARG:HB3	1:A:174:PRO:HG2	1.95	0.49
1:B:578:PHE:N	1:B:579:PRO:CD	2.76	0.49
1:A:484:SER:C	1:A:485:LYS:HD2	2.38	0.49
1:A:748:ARG:NH2	3:A:1039:HOH:O	2.45	0.49
1:B:219:LEU:HD11	1:B:584:LEU:HB3	1.93	0.49
1:B:762:ILE:HG13	1:B:763:GLN:N	2.28	0.49
1:B:204:TYR:HB2	1:B:219:LEU:HB2	1.94	0.49
1:B:578:PHE:HD1	1:B:578:PHE:C	2.21	0.49
1:B:715:LEU:HD11	3:B:1582:HOH:O	2.14	0.48
1:A:846:HIS:HD2	3:A:1583:HOH:O	1.95	0.48
1:B:788:ASP:OD2	3:B:1001:HOH:O	2.20	0.48
1:A:46:PHE:HB3	1:A:77:LEU:HD12	1.96	0.48
1:B:408:LYS:HB2	3:B:1612:HOH:O	2.13	0.48
1:B:578:PHE:HD1	1:B:579:PRO:CD	2.26	0.47
1:A:497:TRP:CE2	1:A:750:PRO:HB2	2.49	0.47
1:A:83:SER:O	1:A:92:SER:OG	2.31	0.47
1:B:282:ILE:HD12	1:B:282:ILE:N	2.29	0.47
1:B:574:GLU:HG2	1:B:580:GLY:O	2.14	0.47
1:A:358:TRP:CE2	1:A:359:ARG:HG3	2.50	0.46
1:B:47:LEU:HD11	1:B:79:GLN:HG2	1.97	0.46
1:B:715:LEU:HD21	3:B:1582:HOH:O	2.15	0.46
1:B:509:ASN:HA	1:B:578:PHE:HE2	1.81	0.46
1:B:419:LEU:HD13	1:B:424:LEU:HD12	1.96	0.46
1:B:724:LEU:CD2	1:B:759:THR:HB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG11	1:B:90:GLY:HA3	1.98	0.46
1:A:569:GLY:HA3	3:A:1260:HOH:O	2.16	0.46
1:A:17:ARG:HG3	1:A:99:ASP:HA	1.99	0.45
1:A:49:LYS:HB3	1:A:49:LYS:HE3	1.68	0.45
1:B:497:TRP:CE2	1:B:750:PRO:HB2	2.52	0.45
1:B:437:LEU:CD1	1:B:450:ALA:HB2	2.47	0.44
1:B:739:GLY:H	1:B:743:TYR:HB3	1.81	0.44
1:A:711:ALA:HA	1:A:715:LEU:HD12	1.98	0.44
1:A:830:GLY:HA2	3:A:1055:HOH:O	2.17	0.44
1:A:745:GLU:HB2	3:A:1039:HOH:O	2.17	0.44
1:B:665:LEU:HD21	1:B:695:LEU:HD13	2.00	0.44
1:B:56:ILE:HD11	1:B:112:VAL:HG23	2.00	0.44
1:B:261:ARG:HD2	3:B:1392:HOH:O	2.17	0.43
1:A:262:PHE:CE2	1:A:553:ARG:NH1	2.86	0.43
1:B:358:TRP:CE2	1:B:359:ARG:HG3	2.53	0.43
1:B:659:LEU:HD11	1:B:665:LEU:CD2	2.49	0.43
1:A:617:SER:O	1:A:620:LYS:HE2	2.18	0.43
1:B:842:ASN:HB2	1:B:857:GLY:HA2	2.00	0.42
1:A:764:THR:O	1:A:768:ILE:HG12	2.18	0.42
1:B:45:GLU:N	1:B:45:GLU:OE1	2.52	0.42
1:A:813:GLU:OE1	1:A:844:SER:OG	2.28	0.42
1:B:290:VAL:HG13	1:B:295:GLY:HA2	2.01	0.42
1:B:227:TYR:CG	1:B:228:PRO:HD2	2.55	0.42
1:A:803:LYS:HE3	1:A:803:LYS:HB3	1.70	0.42
1:B:47:LEU:CD1	1:B:79:GLN:HG2	2.50	0.42
1:B:210:PRO:HG2	1:B:238:THR:HG21	2.01	0.42
1:B:739:GLY:C	1:B:742:GLU:HB2	2.45	0.42
1:B:279:THR:HA	1:B:283:ILE:HD12	2.00	0.42
1:A:49:LYS:HE2	3:A:1182:HOH:O	2.19	0.42
1:B:311:ILE:HD11	1:B:343:LEU:HD22	2.02	0.41
1:B:21:THR:OG1	1:B:80:TRP:HH2	2.02	0.41
1:B:437:LEU:HD11	1:B:450:ALA:HB2	2.01	0.41
1:A:531:VAL:HG22	1:A:552:PHE:CG	2.56	0.41
1:B:79:GLN:O	1:B:80:TRP:CD1	2.69	0.41
1:B:407:GLU:HA	1:B:410:LEU:HD22	2.02	0.41
1:B:737:GLU:C	1:B:743:TYR:HB2	2.45	0.41
1:A:283:ILE:HG12	1:A:766:ILE:HD12	2.02	0.41
1:A:527:MET:HE3	1:A:706:ALA:HB2	2.02	0.41
1:B:705:ILE:HA	1:B:709:LEU:HB3	2.03	0.41
1:A:197:ARG:HH11	1:A:197:ARG:HD3	1.76	0.41
1:A:839:LEU:HD23	1:A:839:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LYS:HD3	1:B:120:GLU:OE2	2.21	0.41
1:A:821:ARG:O	1:A:823:PRO:HD3	2.21	0.40
1:B:419:LEU:HD12	1:B:419:LEU:HA	1.90	0.40
1:B:707:SER:OG	1:B:708:ALA:N	2.53	0.40
1:A:578:PHE:CG	1:A:579:PRO:HD3	2.57	0.40
1:B:837:MET:O	1:B:856:LYS:HA	2.21	0.40
1:A:393:LYS:HE3	1:A:393:LYS:HB3	1.83	0.40
1:A:805:PHE:CZ	1:A:809:LEU:HD11	2.57	0.40
1:A:515:GLN:HG3	3:A:1288:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:ND2	1:B:416:GLN:OE1[1_545]	2.16	0.04
1:B:26:ARG:NH2	1:B:420:ASP:OD2[1_545]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	802/873 (92%)	772 (96%)	30 (4%)	0	100	100
1	B	811/873 (93%)	778 (96%)	32 (4%)	1 (0%)	48	49
All	All	1613/1746 (92%)	1550 (96%)	62 (4%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	738	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	687/739 (93%)	684 (100%)	3 (0%)	84	89
1	B	393/739 (53%)	390 (99%)	3 (1%)	73	80
All	All	1080/1478 (73%)	1074 (99%)	6 (1%)	78	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	280	GLN
1	B	578	PHE
1	B	738	PRO
1	A	134	ARG
1	A	305	ASN
1	A	554	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	301	GLN
1	B	639	HIS
1	B	680	HIS
1	B	761	GLN
1	B	763	GLN
1	B	829	ASN
1	A	214	ASN
1	A	301	GLN
1	A	305	ASN
1	A	317	GLN
1	A	352	GLN
1	A	509	ASN
1	A	515	GLN
1	A	535	ASN
1	A	717	GLN

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Mol	Chain	Res	Type
1	A	761	GLN
1	A	846	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	810/873 (92%)	0.27	39 (4%) 35 37	16, 31, 58, 93	0
1	B	823/873 (94%)	0.12	30 (3%) 46 48	16, 27, 51, 91	0
All	All	1633/1746 (93%)	0.19	69 (4%) 40 42	16, 29, 55, 93	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	855	ALA	8.5
1	A	190	GLY	7.6
1	A	16	ALA	5.6
1	B	383	PHE	5.2
1	B	330	LEU	4.9
1	A	644	TRP	4.6
1	A	746	LEU	4.5
1	A	31	ASP	4.4
1	B	739	GLY	4.3
1	A	383	PHE	4.2
1	A	32	LEU	4.2
1	B	262	PHE	4.1
1	B	190	GLY	3.9
1	B	153	TYR	3.8
1	B	39	VAL	3.8
1	A	410	LEU	3.6
1	B	738	PRO	3.5
1	A	44	SER	3.4
1	B	31	ASP	3.4
1	A	292	THR	3.3
1	A	312	LYS	3.3
1	A	824	GLN	3.3
1	B	644	TRP	3.2
1	A	748	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	395	GLY	2.9
1	A	395	GLY	2.9
1	B	32	LEU	2.8
1	A	743	TYR	2.8
1	B	154	ASN	2.8
1	B	745	GLU	2.8
1	A	81	LEU	2.7
1	A	28	ASN	2.7
1	B	80	TRP	2.7
1	A	262	PHE	2.7
1	A	152	ARG	2.7
1	B	341	TYR	2.6
1	A	797	ARG	2.6
1	B	89	THR	2.6
1	B	746	LEU	2.6
1	B	16	ALA	2.6
1	B	748	ARG	2.5
1	A	87	LEU	2.5
1	A	342	LEU	2.5
1	A	272	GLY	2.5
1	A	412	GLY	2.5
1	B	135	GLY	2.4
1	A	29	VAL	2.4
1	A	267	MET	2.4
1	A	688	LYS	2.4
1	B	384	PRO	2.4
1	A	119	ALA	2.4
1	A	293	THR	2.3
1	B	320	GLU	2.3
1	B	762	ILE	2.3
1	A	745	GLU	2.2
1	A	311	ILE	2.2
1	B	40	VAL	2.2
1	B	41	ASP	2.2
1	A	768	ILE	2.2
1	A	744	GLU	2.1
1	B	152	ARG	2.1
1	A	288	THR	2.1
1	B	338	GLY	2.1
1	A	788	ASP	2.1
1	A	762	ILE	2.1
1	A	118	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	408	LYS	2.0
1	A	287	ARG	2.0
1	B	312	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

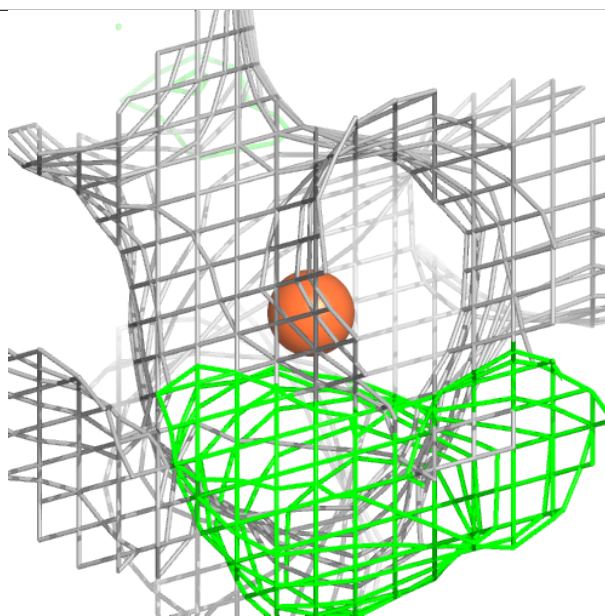
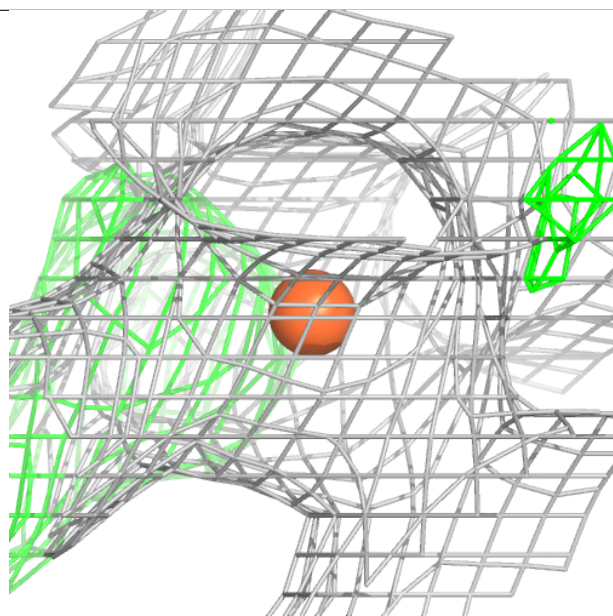
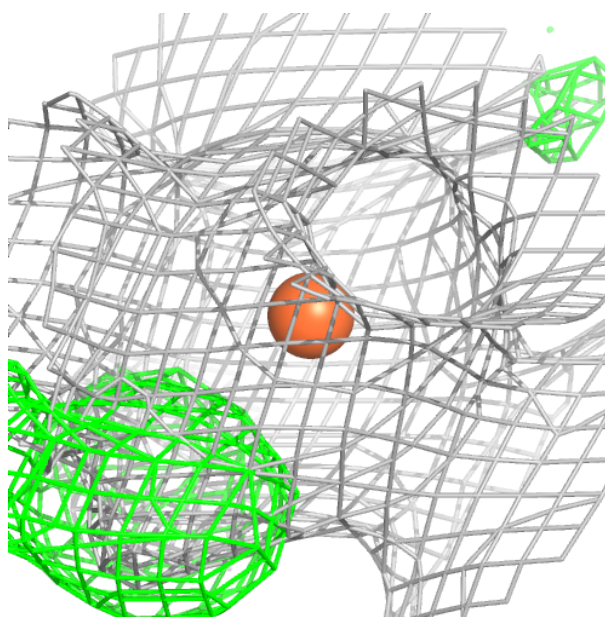
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	901	1/1	0.98	0.02	29,29,29,29	0
2	FE	B	901	1/1	0.99	0.03	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

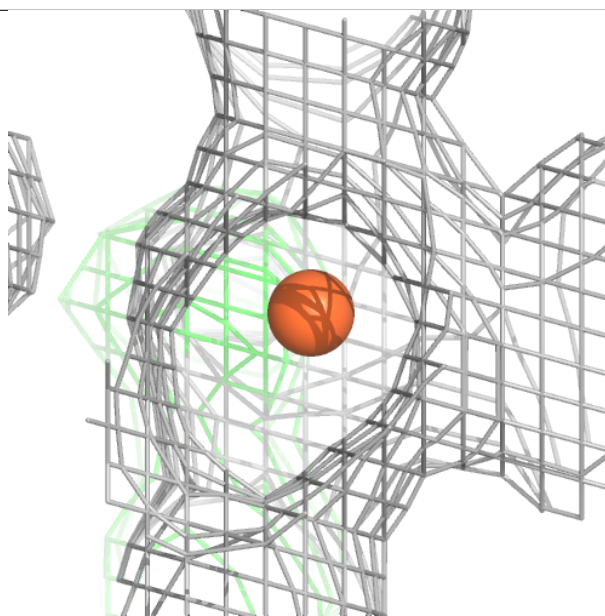
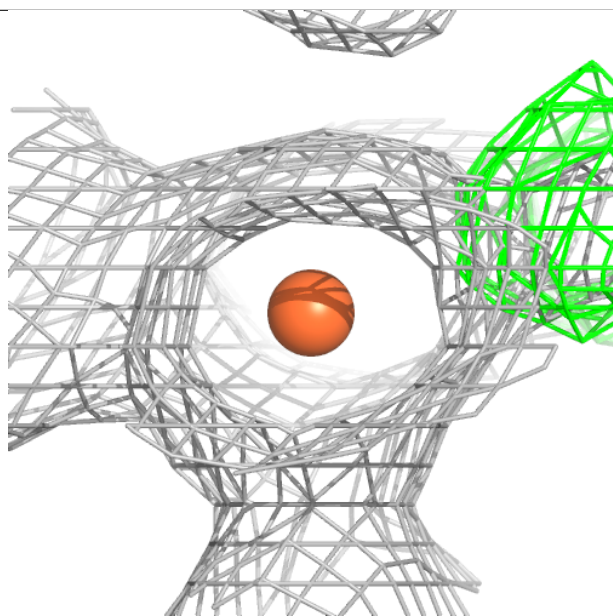
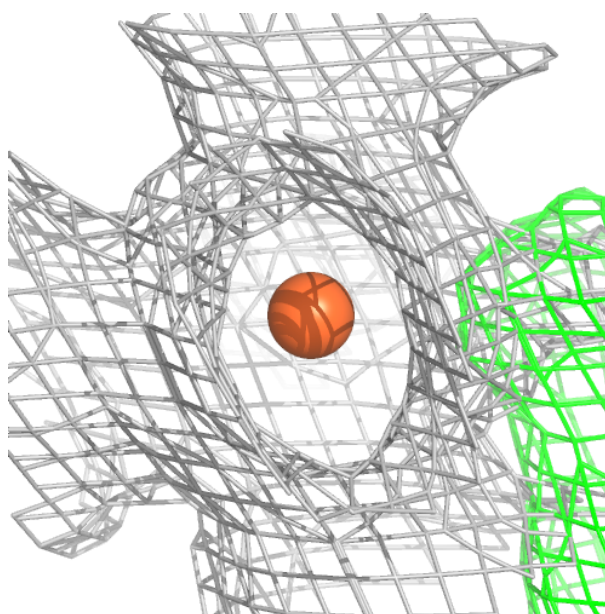
Electron density around FE A 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE B 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.